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FIRST ANNUAL TECHNICAL PROGRESS REPORT
ON

VORTEX SIMULATION OF TURBULENT COMBUSTION

(AFOSR Grant No. 89-0491)

Principal Investigator:

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SUMMARY

During the first year of this activity, we focused on the effect of density variation due to temperature/molecular weight difference and/or heat release in a reacting shear layer in two and three dimensional configurations. In the spatially growing 2D layer, results confirm mixing asymmetry due to density difference between the two streams. A light fast stream has a destabilizing effect on the early stages of development; it promotes early roll-up, induces stronger winding inside the eddies (consistent with linear analysis), and initiates the pairing at earlier stages. However, the overall spatial growth rate of the layer increases as the density ratio becomes higher (heavier fast stream); bigger eddies are formed and pairing is completed faster. In 3D simulations, the density difference between the two streams continues to impart a convection velocity on the structures in the direction of the heavy stream. That influences the evolution of the streamwise mixing modes and spanwise preferential entrainment is observed. Three-dimensional reacting shear layer simulations confirmed earlier 2D observations that although the reaction zone structure depends on the Damkohler number, product distribution is independent of the kinetics parameters and exhibit strong resemblance to the vorticity field. In a simulation of a reacting jet we found that instability suppression due to combustion heat release is weaker for Arrhenius kinetics than for infinitely fast kinetics. Its effects can be weakened further by imposing large initial perturbations.

I. OBJECTIVES

The objectives of this research are:

(1) The development of accurate and efficient numerical methods for the integration of the time-dependent, three-dimensional Navier-Stokes equations, the energy and species conservation equations at high Reynolds and Peclet numbers, moderate Damkohler number, and high rates of heat release. Solution methods are constructed for reacting shear flows at moderate and high Mach numbers.

(2) The investigation of mechanisms of flow-combustion interactions on the basis of the results of the numerical simulations, and the study of how these interactions can be exploited to control burning processes in turbulent shear flows. Numerical simulations results are used to construct physical models which can be used in turbulent combustion closure.

Our work focuses on the development of grid-free, Lagrangian field methods: the vortex element and the transport element methods. To validate these schemes and analyze turbulence-combustion interactions, we perform simulations of reacting shear layers in 2D and 3D. Two combusting flows, distinguished by the distribution of reactants, are analyzed. In the first, the fuel and oxidizer are initially flowing in separate streams. In the second, the fuel and oxidizer are premixed and the second stream contains products. In all cases, we isolate the effects of velocity gradient, density gradient, heat release rate and pressure gradient to determine the role of individual processes in the system. Effort is underway to analyze the role of: (1) large heat release; (2) the Mach number; (3) the chemical kinetics scheme, on the flow field and the combustion process.

II. PERSONNEL

Three graduate students completed their M.Sc. and Ph.D. work during 1989 - 1990:

(1) Knio, Omar, "Three-dimensional Vortex Simulation of Reacting Shear Flow," Ph.D. thesis, M.I.T., June 1990.

(2) Martins, L-P., "Vortex Computations of Axisymmetric High Reynolds Number Flows in Complex Domains," Ph.D. Thesis, M.I.T. June 1990.

(3) Loprinzo, A.J., "Implementation of Multiple Step Chemistry in the Numerical Simulation of Jet Diffusion Flames," M.Sc. thesis, M.I.T. May 1990.

One graduate student is currently working on his Ph.D. under partial support from this contract:

(1) Soteriou, M, "Compressible Vortex Method for the Simulation of High Speed Combustion," 1988 through present.

A half-time postdoctoral research assistant, Omar Knio, is continuing his research on the formulation of three-dimensional vortex methods under the partial support of this grant.

III WORK STATUS

III.1 Baroclinic Effects in a Spatially-Developing Shear Layer.

In this work, we extend our earlier study on the effect of baroclinic vorticity generation due to density variation on the evolution of mixing layers to the case where the layer is growing in space. Two sets of runs were performed for a semiconfined shear layer in a channel with slip walls. In the first, the velocity ratio $U_1/U_2 = 2$ was held constant while the density ratio ρ_1/ρ_2 was varied between 4 and 1/3. In the second set, the velocity ratio was again held constant at 1.6 while the density ratio was varied in such a way as to investigate the effects of the momentum ratio $M_1/M_2 = 1/6, 1, 6$. In all runs the flow was forced at the most unstable frequency and its subharmonic.

Decreasing the density ratio destabilizes the flow. Earlier and more intense roll-up are experienced. This is associated with considerable increase in the stretching of the layers inside the eddies (length of layers approximately doubled between $\rho_1/\rho_2 = 4$ and 1/3). Tongues of irrotational fluid which intrude into the rotational structures penetrate deeper into the large eddies. The early formation of the eddies can be justified by the faster growth of the small perturbation used in the forcing and is consistent with the linear stability analysis which indicates that lower density for the faster stream increases the rate of growth of small perturbations. It is also consistent with the trend in the phase speed of these perturbations which, when measured with respect to the velocity of the mean flow, is in the direction of the heavy stream. These results are observed only at the very early stages of the layer, as expected from the assumptions used in the linear analysis.

Beyond the early stages, decreasing the density ratio leads to the formation of smaller eddies and a delayed progress of pairing of these eddies. The result is a slower expansion of the layer in the cross stream direction, i.e. the spreading rate decreases with decreasing the density ratio. The eddies formed due to the saturation of the fundamental mode continue to move in the direction of the heavy stream with respect to the mean flow, and the interaction between neighboring eddies appear to start earlier, although the pairing process takes longer to reach maturation. Since the velocity ratio was kept constant in these computations, changing the density ratio also changed the momentum ratio. In all cases, however, $M_1/M_2 > 1$ and it was not possible to establish the role of the momentum difference between the two streams on the overall growth rate of the layer.

For this purpose, another set of computations, in which the momentum ratio was varied to cover the entire range $1 > M_1/M_2 < 1$,was obtained. When the momentum ratio was varied systematically, the spreading rate reached a minimum for $M_2/M_1 = 1$ when approached from both ends. This suggests that the momentum ratio is the governing parameter in the spreading rate. As the momentum ratio approaches unity, fluid from each stream finds it exceedingly difficult to intrude into the other stream and the layer centerline (the line passing through the centers of the eddies or that connecting the points moving at the mean velocity) stays parallel to the free streams, the splitter plate, or the channel walls. In this case, the trajectories of the eddies stay almost parallel to each other Without cross stream offset between the centers of neighboring eddies, pairing is inhibited and the spreading rate of the layer is reduced. Thus, the offset angle, or the angle between the centerline of the layer and the splitter plate, is an important parameter which determines the growth rate of the layer.

Results indicate that the offset angle is sensitive to the momentum ratio. At $M_1/M_2 = 1$, the offset angle is almost zero; it is positive if $M_1/M_2 < 1$, and negative for $M_1/M_2 > 1$. As the momentum ratio changes, the layer intrudes into the stream with lower momentum thus increasing this angle. Increasing this angle causes the entire layer to tilt in the same direction and hence changes the entrainment ratio of the two streams. Entrainment is another very important feature of this flow that is significantly influenced by the existence of a non-uniform density field. The results suggest that more light fluid is entrained in the layer and this again is in good agreement with experimental findings. When corrected by the effect of the pressure gradient which develops in the flow, numerical prediction of the entrainment ratio agrees with experimental measurements.

A better understanding of the density effects on the flow can be achieved by examining the vorticity field. In contrast to the uniform density case, vorticity of opposite signs appears across the eddies due to the generation term in the transport equation, leading to strong asymmetry in their structure. By considering the nature of the vorticity generation term together with basic vorticity kinematic principles the creations of positive and negative vorticity across the eddies can be explained. Due to the different signs and position of this newly generated vorticity a net velocity is induced at the center of the eddy. The generated vorticity imposes asymmetry which pushes the structure towards the lower density stream. This asymmetry is responsible for the differential entrainment with a bias towards the light fluid.

During the coming period, the model we be extended to study the effect of baroclinic vorticity generation and volumetric expansion due to combustion heat release in a spatially developing reacting shear layer.

III.2. Flow-Combustion Interactions in a Jet

Vortex simulation, using the transport element method, is applied to study shear flow-combustion interactions in a reacting jet at high Reynolds number. In this study, we used an unsteady, low-Mach number model of combustion in which exothermic energy deposition produces volumetric expansion and baroclinic vorticity, while shear flow instability induces entrainment and a strong strain field. The numerical scheme is a Lagrangian, grid-free, field method in which computations are confined to the vorticity-reaction zone. Solutions are obtained for a two-dimensional flow with a single-step Arrhenius kinetics.

Results show that, as the Damkohler number increases, the reaction zone structure changes from a distributed zone within the cores of the large eddies, which form due to the rollup of the jet vorticity, to a thin zone surrounding their outer edges. The structure of the product distribution, however, remains almost the same, being highest within the cores and falling sharply within the braids, and exhibiting strong similarity to the vorticity distribution. The mechanism leading to this similarity is entrainment. At low Damkohler number, reaction occurs, following the mixing of entrained reactants, inside the eddy core. At high Damkohler number, reaction takes place on the outer edges of the eddies, followed by the entrainment of products towards the eddy center. In both cases, the cores act as exothermic centers which support combustion. With finite-rate kinetics, faster reactions show more robustness towards extinction within zones of high strain rates. We found that instability suppression by heat release is weak at finite-rate kinetics, and can be overcome by forcing the jet at high amplitudes, especially when ignition delay is longer than the time of eddy formation.

During the coming period, we plan to extend the jet model to axisymmetric, spatially developing geometry.

III.3. Burning Enhancement Due to Three Dimensional Structures

The three-dimensional transport element is extended to simulate the unsteady, reacting flow at low heat release. The method is Lagrangian and adaptive. It is based on the discretization of vorticity and species concentration among a number of transport elements of finite overlapping cores. The transport elements are distributed over material surfaces which are advected with the local velocity vector. The tilting and stretching of the vorticity are simulated for using kinematical relationships between its evolution and the deformation of vortex tubes imbedded within the surfaces. The species concentrations are modified according to the local reaction rate, and by diffusion. The scheme employs a vorticity and species concentration redistribution algorithm in two directions: the direction of the vorticity vector, and the direction of maximum strain. Severe and rapid distortions of the material surfaces are thus captured. The method is applied to the study of reacting shear layers in the high Peclet number regime, for a wide range of Damkohler numbers.

Computational results show that product concentration is dominated by the convective field of spanwise and streamwise vortex structures which form by the growth of essential instability of the flow. The rollup of the spanwise vorticity leads to the creation of concentrated vortex cores and braids which join neighboring cores. Entrainment currents associated with these structures force the migration of products from the braids towards the cores, while their induced strain field causes a severe thinning of the braids and of the reaction zone supported therein. Streamwise vortices, which are generated as a result of growth of three-dimensional instability and are intensified by stretch, significantly affect the flow at later stages resulting in substantial deviation from the two-dimensional situation.

The maturation of the streamwise vortices into strong streamwise rods, and the amplification of the translative instability are accompanied by spanwise variations in the reacting field and the formation of mushroom structures. (The mushroom structures describe the deformation of material surfaces around the vortex vortex rods.) Mixing and burning enhancement is achieved through the transverse entrainment fluxes. The entrainment fluxes cause a reorganization of the product distribution such that zones of high product concentration always correspond to zones of high magnitude of vorticity. Products tend to migrate towards the core of the spanwise vortices and the axes of the streamwise vortex rods.

While the product distribution is dictated by the flow, and is insensitive to the value of the Damkohler number, combustion occurs in distributed zones located within the cores of the vortices, and is confined to the initial, well-mixed region. As the Damkohler number increases, complete combustion is achieved within the cores of the vortices causing a migration of the reaction zone towards their outer edges. The motion of the reaction zone towards regions of higher strain rates result in a substantial change in its structure as considerable thinning of the latter is observed.

Work is presently under way to extend the present computations so that pairing among several eddies may be captured. We will be concerned with the generalization of the numerical scheme in order to accommodate high heat release, compressible flow models with complex chemical reactions.

IV. PUBLICATIONS DURING 1988 - 1990

1. Knio, O.M. and Ghoniem, A.F., "Numerical Study of a Three Dimensional Vortex Method," J. Comput. Phys., 86, January 1990, 75-106.(*)[1]

2. Knio, O.M. and Ghoniem. A.F., "Three-dimensional Vortex Simulation of the Rollup and Entrainment in a Periodic Shear Layer," the Journal of Computational Physics, in press.

3. Krishnan, A. and Ghoniem, A.F., "Simulation of the Rollup and Mixing in Rayleigh-Taylor Flow Using the Vortex/Transport Element Method," the Journal of Computational Physics, in press.

4. Ghoniem, A.F. and Heidarinejad, G., "Effect of Damkohler Number on the Reaction Zone in a Reacting Shear Layer," Combust. Flame, in press.

5. Ghoniem, A.F. and Heidarinejad, G. "Effect of Two-dimensional Shear Layer Dynamics on Mixing and Combustion at Low Heat Release," Combust. Sci. Tech., 72, pp. 79-99, 1990. (*)

6. Najm, H. and Ghoniem, A.F., "Vortex Simulation of the Cold Flow Convective Instability in a Dump Combustor," the AIAA Journal, in press.

7. Knio, O.M. and Ghoniem, A.F., "Vortex Simulation of Three-dimensional Reacting Shear Layers," the AIAA Journal, in press, and the 28th Aerospace Sciences Meeting, January, 8-11, Reno, NV, AIAA-90-0150 (*).

8. Ghoniem, A.F., Knio, O.M. and Krishnan, "Lagrangian Simulation of the Initial Stages of a Reacting Jet," the 23rd Symposium (International) on Combustion, July 1990, Orleans, France, proceedings in print.

[1] References marked with (*) are appended to this report.

V. SEMINARS AND LECTURES DELIVERED DURING 1989-1990

During the academic year 1989-1990, the P.I. was on sabbatical Although most of the year was spent in-house to conduct research and supervise graduate students, his outside activities consisted of extended visits to the following organizations:

(1) National Institute of Standards and Technology, Center for Fire Research, October - November 1989.

(2) University of California, Berkeley, February 1990.

(3) University of Nagoya and Institute of Computational Fluid Dynamics, Japan 1990.

The following is a list of seminars delivered during this period:

1. University of Rome Workshop on Fluid Mechanics of Combustion, June 1989.
2. Brown University, October 1989.
3. Ford Motor Company, Meeting on Flow Visualization, November 1989.
4. University of California, Berkeley, CA, February 1990.
5. California Institute of Technology, February 1990
6. University of Southern California, February 1990.
7. NASA Ames Research Center, February 1990.
8. Sandia National Laboratories, February 1990.
9. Lawrence Livermore National Laboratories, February 1990.
10. Nagoya University, 5 - Lecture Course on Computational Combustion, Japan, April 1990.
11. Institute of Computational Fluid Dynamics, Tokyo, Japan, April 1990.
12. Honda Motor Company, Wako, Japan, April 1990.
13. Toyota Motor Company, Nagoya, Japan, April 1990.
14. Nissan Motor Company Research Center, Yokoska, Japan, April 1990.
15. Mitsubishi Heavy Industries, Yokohama, Japan, April 1990.
16. Mazda Motor Company Research Center, Yokohama, Japan, April 1990.
17. SIAM National Meeting, Chicago, July 1990.
18. USSR academy of Sciences, Novosibirsk, USSR, August 1990.
19. Central Institute for Aviation Motors, Moscow, USSR, August 1990.

VI. INTERACTIONS WITH INDUSTRIAL AND GOVERNMENT LABORATORIES DURING 1989 - 1990

During the course of last year, we have started and/or continued collaborative working relations with the following industrial or governmental laboratories.

1. General Electric Research Center and the Gas Research Institute; with Dr. Sanjay Correa on the study of turbulent premixed flames and their instability.

2. Sandia National Laboratory and the Gas Research Institute; with Drs. R. Lucht and John Kelly and their associates on the study of bluff-body diffusion flames.

3. Ford Motor Company; with Mr. C. Kent and L. Ramai, on numerical simulation of flame propagation in enclosures and flow during intake processes.

4. Allison Gas Turbine; with Dr. H. Mongia, on numerical simulation of streamwise vortex structures and their effect on mixing in thrust augmentor sections.

5. National Institute of Standards and Technology; with Dr. H. Baum, on numerical simulation of uncontrolled combustion and plume rise and dispersion.

6. Army Atmospheric Research Laboratory; with Mr. R. Meyers, numerical simulations of flow over complex terrains.

7. Renault Motors in France.

On the international front, the P.I. made extended visits to:

(1) Japan, during which he spend time in Nagoya University, the Institute of Space and Astronautical Sciences and the Institute of Computational Fluid Dynamics in Tokyo. He visited the major Automotive and Aerospace companies and several other universities; and

(2) The Soviet Union. In August, the P.I. participated in a joint workshop held in the Soviet Union between American and Soviet scientists in the field of turbulent subsonic and supersonic combustion. During this period, he visited the USSR Academy of Science in Moskow and Novosbirisk (Institute of Theoretical and Applied Mechanics), Moskow Institute of Aviation, Central Institute for Aviation Motors, Moskow State University, and Moskow Institute of Technology and Physics.